

lattice because of their differing size, causing the lattice constant to be altered. After several stages of data reduction, the WAXS diffraction peaks were fit using the Le Bail fit method in order to determine the lattice constant. Initial results suggest that there may be incorporation of manganese into the UO_2 structure due to a .03 Å decrease in lattice constant, but more data is needed to confirm this. The calcium and magnesium doped samples showed little to no change in the lattice constant, indicating no significant incorporation into the structure. Most importantly, this experiment revealed an artifact of the cleaning process used to remove the bacteria from the sample. It appears the NaOH used to clean the samples is contracting the lattice also by ~.03 Å, but no physical explanation is offered as of yet.

***Evaluating Electrical Conductivity Measurements to Determine Water Flow Rates.** RAY TUGMAN (California State University – Fresno, Fresno, CA); EARL MATTSON (Idaho National Laboratory, Idaho Falls, ID). Centrifuges are used to measure hydraulic properties and solute transport in porous medias. Although the centrifuge is attractive due to the large centrifugal force that it can apply, a major drawback of the centrifuge method is the difficulty of measuring flow rates while the test is in progress. To overcome this limitation, Idaho National Laboratory (INL) scientists are investigating if water flow rate can be determined through the analysis of electrical conductivity measurements in the effluent cup. A prototype electrical conductivity meter was designed and built that can continuously record and transmit electrical conductivity measurements of the effluent while the centrifuge is spinning. The objective of this work is to evaluate the feasibility of the electrical conductivity prototype as to its ability to measure flow rate. If we know the initial volume, the initial electrical conductivity, the electrical conductivity at any given time and the input conductivity, we can calculate the cumulative flux. By plotting the cumulative flux as a function of time, we will produce a graph whose slope is equivalent to the flow rate. In the steady flow tests, the flow rate determined by the cumulative flux of the actual flow rate was constant throughout the experiment and within approximately 2.5% of the actual flow rate. The cumulative flux appears to be noisier in the latter ½ of the data set. In the variable flow test, the calculated cumulative flux predicts the correct shape of the measured cumulative flux curve; however, the calculated cumulative efflux is biased slightly high. This electrical conductivity meter needs further evaluation in the following areas: 1) the effects of mixing in the centrifuge; 2) long term probe drift-how much will the probe drift during experiments lasting several days; 3) optimization of solution initial volumes and concentrations.

The Effects of Hydrologic Conditions on the Distribution of Plant Species in a Mitigated Wetland at Argonne National Laboratory, Illinois. MEAGAN TURNER (Washington State University, Pullman, WA); KIRK LAGORY (Argonne National Laboratory, Argonne, IL). During the construction of the Advanced Photon Source (APS) in 1990 at Argonne National Laboratory in DuPage County, Illinois, three small wetlands totaling 1.8 acres were destroyed. To comply with the no-net-loss policy under the Clean Water Act, a mitigation wetland (Wetland R) was created south of the APS facility. Monitoring of Wetland R began in 1992 and continued annually for five years. In 2002, monitoring started again and has continued through 2007. The purpose of this study was to examine changes in Wetland R with a specific focus on the distribution of species in relation to hydrologic conditions. Percent cover of plant species was determined in 50 quadrats at randomly selected locations along transects throughout the wetland. Each plant species' origin (native, non-native), coefficient of conservatism, and wetland status were recorded. Species were placed in hydrology classes determined by the number of days water was recorded in a quadrat. Overall, the distribution of plant species in 2007 was similar to that in 2005. The distribution of plants according to hydrology was also similar for the two studies except for two species: *Eleocharis erythropoda* and *Boltonia latissuama*. In 2005, 70% of *E. erythropoda* was found in quadrats covered in water greater than 40% of the time. In 2007, 100% of *E. erythropoda* was found in quadrats with no standing water present during 2006 and 2007. In 2005, the majority of *B. latissuama* was found in quadrats covered in water for 1–40% of the time. In 2007, the percentage found in quadrats with no water reached 96%. The hydrology of wetlands strongly affects species composition and richness. It is suggested that Wetland R continued to be monitored for diversity and the distribution of species, especially obligate wetland species, be monitored for changes in response to changing water levels.

The oak savanna. ASHLEY WENTLAND (University of Illinois at Chicago, Chicago, IL); ROD WALTON (Fermi National Accelerator Laboratory, Batavia, IL). The oak savanna, a mixture of prairie grasses, forbs and scattered trees, mainly oaks, was one of the major natural communities

of the Midwest. Today, they are a top concern for restoration. Our objective was to document and characterize the tree population and age structure of the oak savanna by examining relative density, relative frequency, and relative cover for most common species. We conducted tree research in the remnant savanna on Fermi National Accelerator Laboratory's property using the point-centered quarter method. We also prepared soil samples for analyses by First Environmental Laboratories, Inc. in Naperville, Illinois. Ca^{++} and Mg^{++} concentrations were identified for each soil sample. The north side of the savanna has a high tree and vegetation density compared to the south side where there is an abundance of open space and prairie grass. Bur Oak (*Q. macrocarpa*) is by far the most important species in the savanna. However, the basswood (*T. Americana*), white ash (*F. Americana*), and black cherry (*P. serotina*) are slowly dominating the oak savanna at Fermilab, which poses a problem. The data suggest that the north side of the savanna is degraded compared to the description of the healthier side of the savanna. The savanna is being invaded by trees and vegetation and may convert into a woodland if nothing is done. Some possible strategies indicated by our results that may help aid restoration are: removing the invasive tree species, planting more oak species and prairie grasses, and carrying out fires to control the density of vegetation.

Stratigraphic Control on CCl_4 and CHCl_3 Concentrations. KELSEY WINSOR (Smith College, Northampton, MA); GEORGE V. LAST (Pacific Northwest National Laboratory, Richland, WA). An extensive subsurface contaminant plume of carbon tetrachloride (CCl_4) is the focus of a remedial effort in the 200 West Area of Washington State's Hanford Site. Remediation requires a high-resolution model of the region's spatially variable lithofacies and of the effect these units have on CCl_4 migration through the unconfined aquifer. To increase detail of previous models, a transect was chosen along the primary groundwater flow path in the most heavily contaminated area. Borehole logs of wells along this 3.7 km-long transect were systematized and used to create a cross section displaying lithofacies depth and continuity. Natural and spectral gamma geophysical logs were examined to pinpoint the depths of geologic units. Depth discrete concentrations of CCl_4 and its reductive dechlorination product, chloroform (CHCl_3), were overlain on this cross section. Comparison of stratigraphy to contaminant levels shows that peaks in CCl_4 concentration occur in thin, fine-grained layers and that other fine-grained layers frequently form lower boundaries to regions of high concentration. Peaks in CCl_4 concentrations are frequently located at different depths from those of CHCl_3 , suggesting that these concentrations are affected by dechlorination of CCl_4 . Transformation of CCl_4 to CHCl_3 appears to be more prevalent within reduced, iron-containing sediments. Influence of thin, fine-grained layers within the larger aquifer unit indicates that characterization of contamination in this locality should consider subsurface geology with at least as much resolution as provided in this study.

General Sciences

High Order Network Analysis in Power and Pulsed Power of the AGS Main Magnet System. GRACE KING (University of California – Los Angeles, Los Angeles, CA); ARLENE ZHANG (Brookhaven National Laboratory, Upton, NY). Particle accelerator systems like the Brookhaven's Alternating Gradient System (AGS) function on the basis of a high-order network complex of dipole magnets. Comprehensive analysis of this network is essential to the continual success of main magnet system operations. Until now, the limits of current processing technologies have hindered the effective examination of the magnet system's behavior, whose ladder-style characterization can reach hundreds of degrees in its equivalent polynomial form. Previous analysis, which involved the simplification of the circuit system, failed to reflect the nature of its true complexity. Frequency decomposition, aided by the circuit simulation software, Microcap VIII, is a new approach that is able to take advantage of present computer processing capabilities. Presently, distinct circuit models have been simulated and various transient analysis runs have been conducted successfully. Further analysis with the application of transmission-line and ladder-network theory on simulated data should demonstrate the effectiveness of frequency decomposition. The development of this method has greatly facilitated the investigation of present magnet network properties as well as the exploration of new phenomena that may arise from future simulation studies.

Analysis of Mixture Experiments Using Slack Variable and Mixture Approaches. SAMANTHA LANDMESSER (University of Tennessee, Knoxville, TN); GREG F. PIEPEL (Pacific Northwest National

Laboratory, Richland, WA). In a mixture experiment, the response variable depends on the proportions of the components, which must sum to one. Because of this constraint, standard polynomial models cannot be used to analyze mixture experiment data. To get around this, some researchers ignore one of the components and use standard polynomial models in the remaining components. Because the component proportions must sum to one, the ignored component (referred to as the "slack variable" (SV)) makes up the remaining proportion of the mixture. In the literature, there have been many examples of researchers using the SV approach instead of a mixture approach. We have analyzed several of these examples using both approaches. For screening examples, we fit full linear models and identified which components were important using both approaches. In six screening examples, the mixture approach revealed that the SV had a significant effect on the response. For the quadratic examples, we used stepwise regression to develop reduced quadratic models for the SV approach, and partial quadratic mixture (PQM) models for the mixture approach. In three examples, the PQM models identified the SV and/or one of its quadratic blending terms as having a significant effect on the response variable. Hence, by completely ignoring a component's effect on the response, SV analysis carries an inherent risk of wrong conclusions. There are fewer possible reduced quadratic SV models than possible PQM models because the reduced quadratic models are a subset of the class of PQM models. As a result, the PQM models will always fit the data as well as, or better than, the best reduced quadratic SV model. Our research concludes that it is better to analyze mixture experiments using methods specifically developed for them instead of using standard methods with the SV approach.

Planning for the Future: Updating Energy Forecasting

Techniques. CATHERINE SAMPSON (Western Washington University, Bellingham, WA); TODD SAMUEL (Pacific Northwest National Laboratory, Richland, WA). Every year the Energy Information Administration publishes a document known as the Annual Energy Outlook (AEO), which provides analysis and forecasts of world energy markets through the year 2025. The results of this publication are used in the decision making processes of policy makers and public and private investors alike, and are the most comprehensive energy forecasts currently available. However, the National Energy Modeling System (NEMS), the program used to produce these forecasts, is riddled with minor flaws that may have major impacts on the applications of the AEO results. Though built using a detailed, modular structure, NEMS can only be run deterministically on a scenario by scenario basis. Further, NEMS models display an asymmetric loss function, making the results ambiguous to users whose loss function is not identical to that of modelers'. That is why the Department of Energy and the National Renewable Energy Laboratory are commissioning a new model for forecasting energy use. Known as the Stochastic Energy Deployment System (SEDS), this model will improve on current energy modeling mechanisms by providing for full probabilistic treatment of uncertainties. SEDS is in development under experts from several national laboratories, and will be designed on Analytica, a commercially available software package offering a user-friendly format. Hopefully, SEDS will be able to provide forecasts with better representations of the various possible futures of energy markets than are currently available.

Testing the Multiwavelet Representation of Functions. OWEN WORLEY (Dartmouth College, Hanover, NH); GEORGE FANN (Oak Ridge National Laboratory, Oak Ridge, TN). The multiwavelet transformation of functions is one of the most promising methods for analyzing and performing operations on them. The multiwavelet expansion represents functions in terms of a basis of discontinuous multiwavelet functions, which are nonzero over a unit domain. In particular, representations of the Green's function of operators of partial differential equations, constructed in multiwavelet bases, can be proven, in many cases, to be sparse and nearly diagonal. Thus, the computational complexity of the application of these operators is linear or nearly linear with respect to the problem size, and so is very attractive as a method of solution. As in the development of any complex software, testing must be done to assure that the transformed function behaves correctly with respect to basic algebraic and calculus operations. This testing is done by creating and inputting a variety of functions into a program, calculating the multiwavelet representation of these functions, applying a number of operators to both the original and transformed functions, and comparing the results, demonstrating that operating on the multiwavelet representation is numerically stable and achieves the required accuracy. Said testing demonstrated that the transformed functions do behave correctly with respect to the algebra and calculus operations tested to a high degree of accuracy. Also, as the tests

were scaled to higher numbers of processors, the completion times decreased in a smooth log curve. These results were expected, but in obtaining them, debugging was performed and problems were identified and worked around. Further testing should be performed on functions represented with a higher wavelet order, and testing should generally be done as the code is modified and improved. The Joule program, written by George Fann and Robert Harrison, performs the multiwavelet transformation which is tested. The paper, Adaptive Solution of Partial Differential Equations in Multiwavelet Bases, by B. Alpert et al, provides background on multiwavelet transformations.

Materials Sciences

The Effects of Amorphous Carbon Coating of Standard Modified Graphite and Soft Carbon on Anode Properties for Li Ion Batteries. DAVID ABRAM (University of Illinois, Urbana, IL); JUN LIU (Argonne National Laboratory, Argonne, IL). Hybrid electric vehicles are gaining popularity to increase fuel efficiency and lessen dependency on oil. The battery used is predominantly nickel metal hydride, but there is a push to use Li ion batteries due primarily to their higher gravimetric and volumetric energy density. Improvements in anode quality can be made, and six Hitachi anodes consisting of blank soft carbon and surface modified graphite as well as the same materials with an amorphous carbon coating were examined. Formation cycles were run for half cells against lithium and full cells against $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}/\text{3O}_2$. Hybrid pulse power characterization tests were run to determine the area specific impedance at various depths of discharge for the full cells. The half cell formation cycles showed that the charge capacity neared the theoretical capacity limit for graphite of 372 mAh/g while the capacity was much lower for soft carbon at around 220 mAh/g. The coating increased the capacity by 4% and reduced the area specific impedance by 36% for the soft carbon. The effects at the same particle size of 20 microns were inconclusive for the graphite, but there was a 25% decrease in area specific impedance when the particle size was decreased. The effect of the coating on the performance of the soft carbon was visibly beneficial while the effects for the graphite may have been due more to particle size. A new test involving a 10 micron graphite blank and a larger electrode area will be done in the future to closer examine the phenomena.

High Activity Fuel Cell Catalysts via Mesoporous Nanocomposite

Polymers. GREGORY BAKER (Pennsylvania State University, University Park, PA); ERIC COCHRAN (Ames Laboratory, Ames, IA). Hydrogen fuel cells have the potential to improve the way we propel our vehicles. Catalyst particles within cathode catalyst layer (CCL) promote the reaction of protons, electrons, and oxygen, producing water, which must be removed. The current CCL design suffers from poor mass transport properties, limiting the efficiency of the present-day hydrogen fuel cell. The current structure is a combination of different materials put together to achieve these goals but lacks the order needed to achieve the desired efficiency. In this research, we investigated the development of a novel CCL design that will significantly increase the transport of reactants to active catalyst sites. The first step towards this design was the synthesis of a new catalyst support, based on single-wall carbon nanotubes (SWCNTs), that integrates electron and proton conductivity into a single particle. First, pristine SWCNTs were functionalized with an aniline derivative compound using a solvent free technique. Then, azide-terminated polystyrene was "click-coupled" to the alkyne group. This SWCNT-graft-polystyrene was then sulfonated; this created negatively charged regions in the polymer, which facilitated the deposition of platinum nanoparticles through the reduction of platinum salts. After sulfonation the polymer is also proton-conductive. Thermogravimetric analysis analyzed the effectiveness of the grafting reactions. Nuclear magnetic resonance spectroscopy demonstrated that the proper products were prepared during the synthesis of the aniline derivative and also to ensure that azide terminated polystyrene was achieved. Transmission electron microscopy determined the effectiveness of the decoration with platinum.

Oxidation Characterization of Chromium Tungsten Niobium

Superalloys. AMANDA BASTIDOS (University of Texas at El Paso, El Paso, TX); KEN NATESAN (Argonne National Laboratory, Argonne, IL). The past 50 years of metallurgical and materials engineering has brought about much more technologically advanced materials and alloys. One of the dilemmas with current alloys used in high temperature environments is the temperature limit seems to peak at 1,000°C. The overall goal of this research project is to characterize the oxidation layers of a chromium tungsten niobium (CrWNB) superalloy in short term oxidation (STO) experiments and long term oxidation (LTO) experiments in high temperature environments (700–1,400°C).